

1,1,1,3,3,3-Hexafluoropropan-2-yl trifluoroacetate
42031-15-2 | DTXSID80340673

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 1.29

Global applicability domain: Inside

Local applicability domain index: 9.44e-01

Confidence level: 5.75e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Ethane</div> <div>Measured: 0.42</div> <div>Predicted: 1.04</div>	<div>Image not found</div> <div>Chloromethane</div> <div>Measured: 1.39</div> <div>Predicted: 1.58</div>	<div>Image not found</div> <div>Dimethyl ether</div> <div>Measured: 1.37</div> <div>Predicted: 1.58</div>
<div>Image not found</div> <div>Nitromethane</div> <div>Measured: 2.53</div> <div>Predicted: 1.63</div>	<div>Image not found</div> <div>Propane</div> <div>Measured: 0.97</div> <div>Predicted: 1.60</div>	